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Interpretation of Survey Water Quality Data

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FORMAT FOR ACQUIRING RAPID DATA ANALYSIS CAPABILITIES OF STORET DATA: Manipulation of National Eutrophication Survey Water Quality Data

by

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16. ABSTRACT

As an integral part of the National Eutrophication Survey, a program initiated in 1972 in response to an Administration commitment to investigate the threat of accelerated eutrophication to freshwater lakes and reservoirs, the Water and Land Quality Branch, Monitoring Operations Division, Environmental Monitoring and Support Laboratory-Las Vegas, has collected water quality information from selected lakes throughout the contiguous United States. Water quality data are categorized and stored using a U.S. Environmental Protection Agency central computer-oriented system, STORET (STOrage and RETrieval).

The data processing and analytical requirements of the Branch were not met by the program options internal to the STORET system. A need for raw data conversions in STORET to some other accessible form was recognized. With the cooperation of the Data Services Branch, Office of Program Management and Support of the same laboratory a job control language package, "STORET.TO.WYLBUR." was written for conversion of raw data in STORET into a standardized format for statistical evaluation and manipulation of Survey data. This data analysis scheme may be ideal for general use as another program option internal to the STORET system.

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INTRODUCTION

The National Eutrophication Survey was initiated in 1972 in response to an Administration commitment to investigate the nationwide threat of accelerated eutrophication to freshwater lakes and reservoirs.

The Survey was designed to develop, in conjunction with State environmental agencies, information on nutrient sources, concentrations, and impact on selected freshwater lakes as a basis for formulating comprehensive and coordinated national, regional, and State management practices relating to point source discharge reduction and nonpoint source pollution in lake watersheds.

As a principal participating staff of the National Eutrophication Survey,* the Environmental Monitoring and Support Laboratory-Las Vegas' Water and Land Quality Branch of the Monitoring Operations Division has collected water quality data from more than 800 selected lakes throughout the contiguous United States. To date, the Survey has yielded more than two million data points.

Analyses of these water quality data address problems unique to lakes and not amenable to those computer programs available in the U.S. Environmental Protection Agency's STORET (STOrage and RETrieval) system.

Consequently, a job control language package, "STORET.TO.WYLBUR," was developed to convert raw data in STORET to a standardized format for statistical evaluation and manipulation of Survey data.

"STORET.TO.WYLBUR" has proven to be a very effective means for acquiring rapid data analysis capabilities of STORET data and may be implemented with facility by both experienced and relatively inexperienced computer programmers.

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*The Special Studies Branch, Criteria and Assessment Division, Corvallis Environmental Research Laboratory, Corvallis, Oregon is also a principal participating staff of this project. The Corvallis laboratory was primarily responsible for the collection of municipal sewage treatment plant and tributary water quality data (USEPA 1975).

CONCLUSIONS AND RECOMMENDATIONS

The "STORET.TO.WYLBUR" program has satisfied the Water and Land Quality Branch's additional requirements and is easily used by most computer personnel. This data analysis scheme may well be ideal for general use. It is recommended that the program be added as another program option internal to the Agency's STORET system and the supporting documentation be generated to assist those wishing to use this computer program.

PURPOSE

The purpose of this report is to demonstrate a system for a STORET user to acquire rapid and flexible data analysis capabilities with minimal effort. The data management scheme outlined is for the use of organizations which have, or will have, a data base in STORET and require programming options beyond those available in STORET.

The following definitions of terms may be helpful to enhance the reader's comprehension:

STORET (STOrage and RETrieval): a central computer-oriented system used by the Agency to categorize, store, and retrieve water quality data.

PGM=RET: a STORET program command calling for a variety of retrieval programs internal to STORET.

MORE File: an assigned name for a disk file created by PGM=RET retrieval which contains condensed IBM (International Business Machines) hexadecimal output (USEPA 1974, Volume 2, Chapter 10, Section M).

WYLBUR: an assigned name for a text "editor" and remote job entry facility available through OSI (Optimum Systems Incorporated).

EDIT: a format compatible with the WYLBUR text-editing system available through OSI.

SAS (Statistical Analysis System) and BIOMED (Biomedical Statistical Computer Programs): two software packages which allow convenient implementation of various statistical techniques.

The procedures involved in implementing this scheme were designed to enable users with various levels of systems expertise to use them. To best operate this system, a user must understand the mechanics of conducting STORET retrievals, particularly PGM=RET, its associated options, and the more common WYLBUR editing commands. The ability to tailor the raw data retrievals from STORET will help appreciably in preparing data for further analysis.

HISTORICAL BACKGROUND

In early 1974, the only computer operation within the Water and Land Quality Branch consisted of STORET (lake) data retrievals via a remote terminal (WYLBUR). Because the data processing and analytical requirements were not satisfied by the program options internal to the STORET system, a serious need to convert the raw data in STORET to some other accessible form was recognized.

The Branch alerted the Laboratory's data services staff (Data Services Branch, Office of Program Management and Support) to this problem and requested their assistance. As a result, a job control language (JCL) package, "STORET.TO.WYLBUR," was written. This program contains the appropriate IBM JCL and FORTRAN (FORmula and TRANslation, a computer language) programming (Friedland 1974) for conversion of the PGM=RET output, or raw data retrieval of STORET, into an acceptable input form for use with so-called packaged programs (e.g., SAS, BIOMED) or user-created programs.

After a short training course on SAS, Branch personnel were able to make data evaluations. Within about 3 months, the same personnel could handle most analytical requirements with ease. Using "STORET.TO.WYLBUR" in conjunction with SAS has proven to be a powerful and highly flexible tool for data analysis.

PROGRAM SUMMARY

Initially, STORET retrieval data are transferred into a MORE File by PGM=RET. "STORET.TO.WYLBUR" accesses this file and converts it to standard card-images and then into EDIT format. Data are then accessible to the WYLBUR user for input into mathematical packages such as SAS, BIOMED, etc., and subsequently are easily analyzed (or merged with other data files) in accordance with the unique requirements of a given research program. Both novice and expert users are able to use this data handling method successfully.

CONCEPT OF DATA ANALYSIS

Generally, data analysis operations within the Branch are divided into three primary areas of involvement, as shown in Figure 1. These areas are:

(1) STORET - used primarily as a data storage facility. Except for transfer of raw data in the "STORET.TO.WYLBUR" operation, minimal use is made of the programs internal to STORET.

(2) "STORET.TO.WYLBUR" - converts data into EDIT format from the MORE File generated by the STORET raw data retrieval. The stylized output format is compatible with packaged programming or user-created programming.

(3) SAS - used for its extensive ability to manipulate and analyze data (equivalent to FORTRAN) and to perform numerous statistical procedures which generate plots, implement regression analyses, etc.

Other operations include merging or concatenation of other files (block 4.) with the STORET data (block 1.). SAS can also generate data cards to be used in other programs (block 5.).

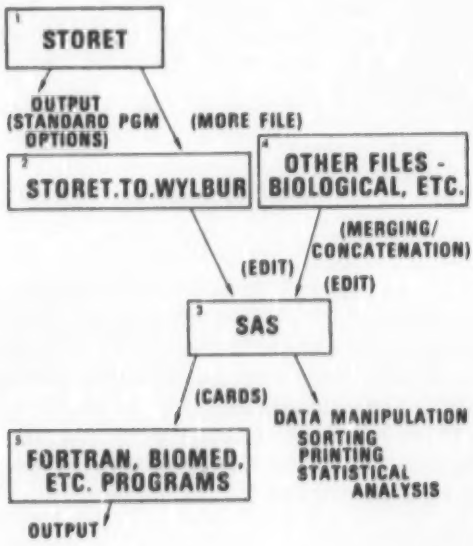

Figure 1. Output flow diagram demonstrating data processing logic.

"STORET.TO.WYLBUR"

USING "STORET.TO.WYLBUR"

The necessary changes for setting up a job are located in three areas of the JCL package, as shown in Figure 2.

```
1.      //IIIWY JOB (AAAA,BIN,01,01,01),' STR-TO-WYL',MSGLEVEL=(1,1)
2.      // EXEC WQDIST
3.      //DIST.CARDFD DD *
4.      PGM RET,PURP=104/EPA,A 11EPALES,MORE=4,RMT 35,B P,
5.      S=380000,S=380499,
6.      P=671,P=665,
7.      T=77777702,
8.      PRT=NO,
9.      // EXEC FORTGLG PARM='NOMAP'
10.     //LKED.SYSIN DD DSN=CNA805.RWT.RDSTOR,
11.     //    UNIT=3330,VOL=SER=TS0004,DISP=SHR
12.     //GO.FT15F001 DD DSN=&FCF,DISP=(OLD,DELETE)
13.     //GO.FT12F001 DD DSN=&LAKFIL,DISP=(NEW,PASS),UNIT=SYSDA,
14.     //  SPACE=(TRK,(25,10)),DCB=(RECFM=FB,LRECL=80,BLKSIZE=1680)
15.     //GO.SYSIN DD *
16.     02 NUMBER OF PARAMETERS RETRIEVED IN 1-2 (1-50)
17.     // EXEC EDSCARDS,NAME='CNA805.RWT.DATA.SET',DISK=TS0001,TYPE=OLD
18.     //CARDS DD DSN=&LAKFIL,DISP=OLD
```

Figure 2. Listing of "STORET.TO.WYLBUR"

On Line 1 is the job card which must be adjusted to comply with the initials and account of each user (see OSI 1973, p. 2-1). The second segment to be changed is Lines 4-8, the STORET retrieval coding for the data that are to be converted. If "PRT=NO" (a STORET program command meaning "do not print") is not included, STORET raw data printout will also be generated. On Line 16, the number of parameters found in the STORET coding is given. Line 17 identifies the disk file where the converted data are written and the file name.

Disk and data set name (Line 17) must be adjusted to fit individual requirements as shown below:

```
17 //EXEC EDSCARDS, NAME='CNAA.BBB.CCC',DISK=TSOXXX,TYPE=OLD

        where       AAA = Account No.
                    BBB = Initials
                    CCC = Data Set Name
                    XXX = Volume Used
```

Since the file type is old, a dummy file with the file name assigned by the user should be saved on the disk pack indicated. A copy of the program entitled "&CNA805.RWT.STORET.TO.WYLBUR" is currently available to interested persons on TSØ001 (one of 16 on-line disk packs currently available through OSI).

"STORET.TO.WYLBUR" OUTPUT

The output of "STORET.TO.WYLBUR" written onto a disk pack follows the format shown in Figure 3.

					Station	Date	Time	Depth	Sequence
0.170	0.260	0.000	0.000	0.000	0.00038010174	430	920		01
0.161	0.245	0.000	0.000	0.000	0.00038010174	430	920		51
0.160	0.243	0.000	0.000	0.000	0.00038010174	430	920		151
0.155	0.239	0.000	0.000	0.000	0.00038010174	430	920		231
0.279	0.283	0.000	0.000	0.000	0.00038010174	7171	120		01
					⋮				

Figure 3. The data set created by "STORET.TO.WYLBUR" on TSØ002

Because only a maximum of six parameters can be written per line, a sequence number is given at the end of each line to indicate whether it is the first, second, or a succeeding line of information for a given station.

Each parameter result field is 10-columns wide. The following are listed at the end of each line: the station STORET number in columns 61-66; year, 67-68; month, 69-70; date, 71-72; time of day, 73-76; depth, 77-79; and sequence in column 80.

Because missing values are represented by "-123.000," it is necessary to replace these numbers with a string of eight blanks using the WYLBUR "CHANGE" command before making use of these data sets. The programming allows up to 50 parameters to be converted to EDIT format in any one given run.

Advantages

(1) Anyone who can set up a STORET raw data retreival will have minimal problems in converting it into EDIT format on the OSI computer systems.

(2) The data output of "STORET.TO.WYLBUR" has a formalized structure which provides a data file on which other programs (e.g., user-written, BIOMED, SAS) can operate.

(3) Minimal knowledge of IBM JCL is required. The "STORET.TO.WYLBUR" program is ideal for users who have neither time nor long-term requirements to learn the intricacies of IBM JCL.

DISADVANTAGES

(1) Parameter order must be clearly determined on the data file created, or gross errors may occur in subsequent analyses.

(2) Large "STORET.TO.WYLBUR" data files are expensive to manipulate using the WYLBUR editor.

A WORD ABOUT SAS

SAS is the principal software package used by the Branch, and its capabilities can be clearly stated. First of all, SAS is a unified system of data manipulation, editing, and statistical analysis (Service 1972). Programming and assignment statements are designed to enable the user to effectively modify data prior to final analysis and display.

Statistical analysis, plotting, and sorting can usually be implemented using only several lines of coding associated with "PROCEDURE" statements. Subsetting, concatenation, and data-set merging have proven to be invaluable tools in data manipulation available in SAS. In fact, SAS has been used extensively to merge water quality information originating in STORET with biological information to create needed data files.

SAS may also be used to process information with the subsequent output passed from the system into card format for input into other software packages or user-written programming.

A sample SAS program built around a data file created by "STORET.TO.WYLBUR" is shown in the Appendix. The output of the program is also included.

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Service, Jolayne. 1972. A User's Guide to the Statistical Analysis System. (Based on Statistical Analysis System Manual prepared by A. J. Barr and J. H. Goodnight). Student Supply Stores, North Carolina State University, Raleigh, North Carolina.

U.S. Environmental Protection Agency. 1974. Handbook - Water Quality Control Information System - STORET. Volume 2, Chapter 10, Section M. Washington, D.C.

_____. 1975. National Eutrophication Survey Methods 1973-1976. National Eutrophication Survey Working Paper No. 175. National Environmental Research Center, Las Vegas, Nevada, and Pacific Northwest Environmental Research Laboratory, Corvallis, Oregon.

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_____. 1975. User's Manual for EPA Scientific Applications Software. Washington, D.C.

APPENDIX

"STORET.TO.WYLBUR" - A SAMPLE RUN

1. The program (&CNA805.RWT.STORET.TO.WYLBUR ON TSØ001) ran:

```
//RWTWY JOB (A805,BIN,01,01,01), 'STR-TO-WYL,MSGLEVEL=(1,1)
// EXEC WQDIST
//DIST.CARDFD DD *
PGM RET,PRUP=104/EPA,A 11EPALES,MORE=4,RMT 35, B P,
 S=380000,S=380499,
P=671,P=665,
T=77777702,
PRT=NO,
// EXEC FORTGLG,PARM='NOMAP'
//LKED.SYSIN DD DSN=CNA805.RWT.RDSTOR,
//    UNIT=3330,VOL=SER=TS0004,DISP=SHR
//GO.FT15F001 DD DSN=&FCF,DISP=(OLD,DELETE)
//GO.FT12F001 DD DSN=&LAKFIL,DISP=(NEW,PASS),UNIT=SYSDA,
//  SPACE=(TRK,(25,10)),DCB=(REDFM=FB,LRECL=80,BLKSIZE=1680)
//GO.SYSIN DD *
02  NUMBER OF PARAMETERS RETRIEVED IN 1-2 (1-50)
// EXEC EDSCARDS,NAME=CNA805.RWT.DATA.SET',DISK=TS0002,TYPE=OLD
//CARDS DD DSN=&LAKFIL,DISP=OLD
```

2. Segment of data set written (note that the data set is a standard WYLBUR File and is accessed into working memory by the "USE" command):

Data Set Name: DATA.SET Location: TSØ002

```
0.170   0.260   0.000   0.000   0.000   0.00038010174 430 920  01
0.161   0.245   0.000   0.000   0.000   0.00038010174 430 920  51
0.160   0.243   0.000   0.000   0.000   0.00038010174 430 920 151
0.155   0.239   0.000   0.000   0.000   0.00038010174 430 920 231
0.279   0.283   0.000   0.000   0.000   0.00038010174 7171120  01
0.277   0.292   0.000   0.000   0.000   0.00038010174 7171120  51
0.307   0.326   0.000   0.000   0.000   0.00038010174 7171120 151
0.274   0.318   0.000   0.000   0.000   0.00038010174 7171120 201
0.220   0.275   0.000   0.000   0.000   0.00038010174 9171410  01
0.204   0.245   0.000   0.000   0.000   0.00038010174 9171410 151
0.193   0.245   0.000   0.000   0.000   0.00038010174 9171410 271
```

3. The SAS program below is built around the preceding data set. Check the external copy command in the OSI Manual for rapid combining methods of pre-existing programming and data files.

```
//RWT JOB (A805,45,1,1),'SAS RUN',MSGLEVEL=(0,0)
// EXEC SAS
//SAS.SYSIN DD *
TITLE 'ORTHOPHOSPHATE VS TOTAL PHOSPHORUS FOR SELECTED LAKES';
DATA RAW;
INPUT PORTHO 1-10 PT 11-20;
CARDS;
     0.170     0.260     0.000     0.000     0.000     0.00038010174 430 920  01
     0.161     0.245     0.000     0.000     0.000     0.00038010174 430 920  51
     0.160     0.243     0.000     0.000     0.000     0.00038010174 430 920 151
     0.155     0.239     0.000     0.000     0.000     0.00038010174 430 920 231
     0.279     0.283     0.000     0.000     0.000     0.00038010174 7171120  01
     0.277     0.292     0.000     0.000     0.000     0.00038010174 7171120  51
     0.307     0.326     0.000     0.000     0.000     0.00038010174 7171120 151
                                       .
                                       .
                                       .
     0.193     0.245     0.000     0.000     0.000     0.00038010174 9171410 271
     0.147     0.261     0.000     0.000     0.000     0.00038010274 430 945  01
     0.138     0.247     0.000     0.000     0.000     0.00038010274 430 945  81
     0.273     0.377     0.000     0.000     0.000     0.00038010274 7171030  01
     0.280     0.314     0.000     0.000     0.000     0.00038010274 7171030  51
     0.281     0.319     0.000     0.000     0.000     0.00038010274 7171030 171
     0.088     0.224     0.000     0.000     0.000     0.00038010274 9171455  01
PROCEDURE PRINT;
PROCEDURE PLOT;
PROCEDURE CORR;
PROCEDURE REGR; MODEL PROTHO=PT;
/*
```

4. Following are illustrations of the output generated by the preceding program. The results of the commands PROCEDURE PRINT;, PROCEDURE PLOT;, PROCEDURE CORR;, PROCEDURE REGR; MODEL PROTHO=PT;, can be fetched using "FETCH XXX DDN= FT03F001" where XXX is the job number. This output demonstrates the capabilities of the SAS "PROCEDURE" statements and was a modified program exampled (Service 1972).

ORTHOPHOSPHATE VS TOTAL PHOSPHORUS FOR SELECTED LAKES

```
TITLE 'ORTHOPHOSPHATE VS TOTAL PHOSPHORUS FOR SELECTED LAKES';
DATA RAW;
INPUT PORTHO 1-10 PT 11-20;
CARDS
```

106 OBSERVATIONS IN DATA SET RAW 2 VARIABLES

PROCEDURE PRINT;

ORTHOPHOSPHATE VS TOTAL PHOSPHORUS FOR SELECTED LAKES

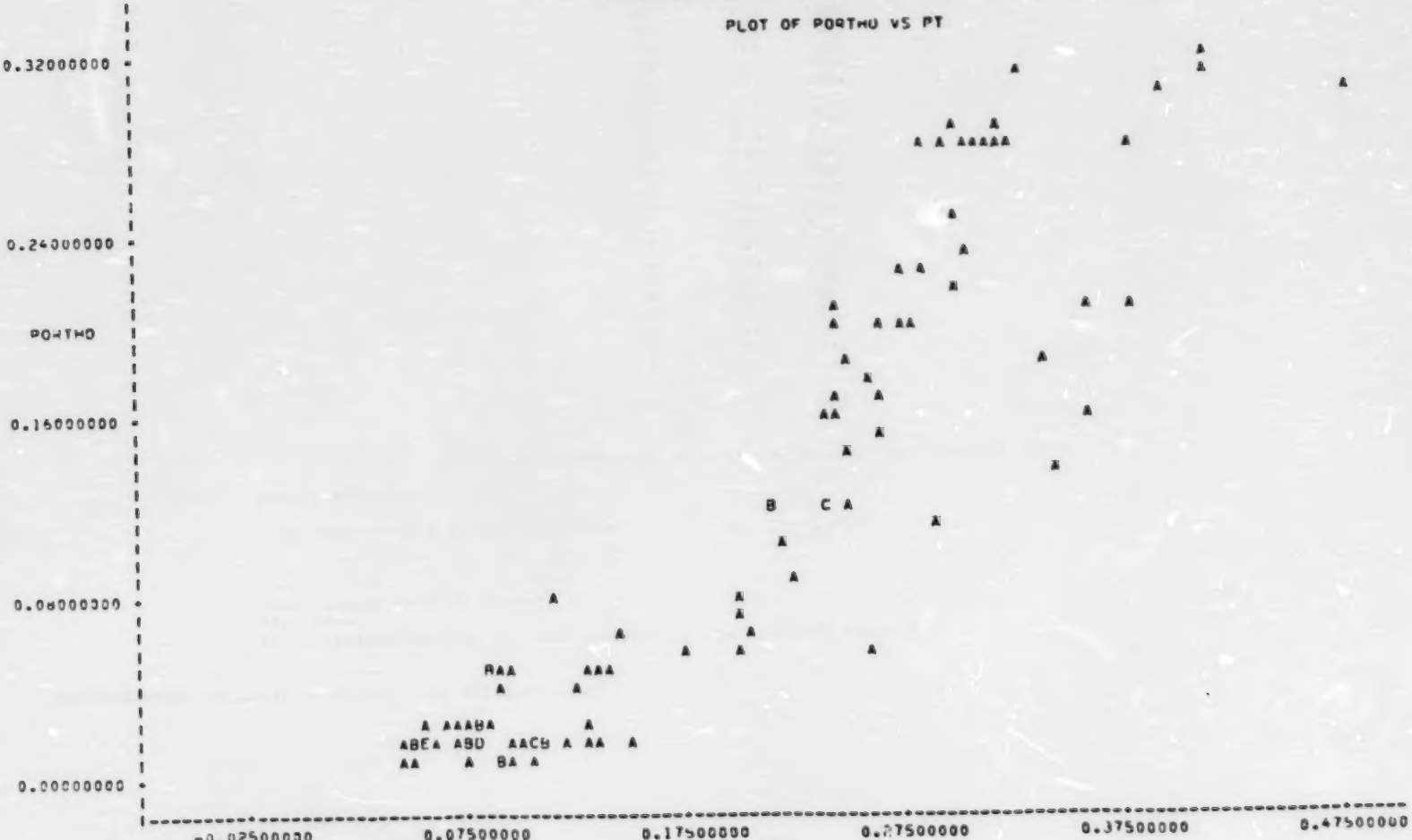
OBS	PORTHO	PT
1	.170	.260
2	.161	.245
3	.160	.243
4	.155	.239
5	.279	.283
6	.277	.292
7	.307	.326
8	.274	.318
9	.220	.275
10	.204	.245
11	.193	.245
12	.147	.261
13	.138	.247
14	.273	.377
15	.280	.314
16	.281	.319
17	.088	.224
18	.097	.216
19	.119	.237
20	.117	.237
21	.119	.236
22	.304	.477
23	.317	.412

.
.
.

PROCEDURE PLOT:

ORTHOPHOSPHATE VS TOTAL PHOSPHORUS FOR SELECTED LAKES

PLOT OF PORTHO VS PT



LEGEND: A = 1 OBS , B = 2 OBS , ETC.

ORTHOPHOSPHATE VS TOTAL PHOSPHORUS FOR SELECTED LAKES

14:18 THURSDAY, OCTOBER 9, 1975

ORTHOPHOSPHATE VS TOTAL PHOSPHORUS FOR SELECTED LAKES

	N	SUM	MEAN	MIN VALUE	MAX VALUE	CORRECTED SS	STANDARD DEV
ORTHO	106	10.99700000	0.10374528	0.00600000	0.31700000	1.08141012	0.10148478
T	106	19.64900000	0.18536792	0.04100000	0.47700000	1.27834065	0.11033690

ORTHOPHOSPHATE VS TOTAL PHOSPHORUS FOR SELECTED LAKES

N = 106 CORRELATION COEFFICIENTS / PROB > |R| UNDER HO: RHO=0

	PORTHO	PT
ORTHO	1.000000	0.921752
	0.0000	0.0001
T	0.921752	1.000000
	0.0001	0.0000

PROCEDURE REGH: MODEL PORTHO=PT:

PROC REGH : ORTHOPHOSPHATE VS TOTAL PHOSPHORUS FOR SELECTED LAKES

DATA SET : RAW NUMBER OF VARIABLES = 2 NUMBER OF CLASSES = 0

VARIABLES : PORTHO PT

ORTHOPHOSPHATE VS TOTAL PHOSPHORUS FOR SELECTED LAKES

ANALYSIS OF VARIANCE TABLE . REGRESSION COEFFICIENTS . AND STATISTICS OF FIT FOR DEPENDENT VARIABLE PORTHO

SOURCE	DF	SUM OF SQUARES	MEAN SQUARE	F VALUE	PROB > F	R-SQUARE	C.V.
REGRESSION	1	0.91879534	0.91879534	587.61393	0.0001	0.84962709	38.11492 %
ERROR	104	0.16261479	0.00156360			STD DEV	PORTHO MEAN
CORRECTED TOTAL	105	1.08141012				0.03954243	0.1037 5

SOURCE	DF	SEQUENTIAL SS	F VALUE	PROB > F	PARTIAL SS	F VALUE	PROB > F
PT	1	0.91879534	587.61393	0.0001	0.91879534	587.61393	0.0001

SOURCE	B VALUES	T FOR HO:B=0	PROB > |T|	STD ERR B	STD B VALUES
INTERCEPT	-0.05340699	-7.08762	0.0001	0.00753525	0.0
PT	0.84778571	24.24075	0.0001	0.03497358	0.92175218